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Electron transport in a mesoscopic wire: the charging and exchange interaction effects

V. A. Sablikov and S. V. Polyakov
Institute of Radio Engineering and Electronics, RAS,
Moscow District, Fryazino, 141120, Russia

Abstract. We have shown that the difference of the chemical potentials appears between a semiconductor quantum wire and electron reservoirs. It can be comparable with the Fermi energy of electrons. Due to the chemical potential difference the electron density is redistributed between the wire and reservoirs and the wire acquires the charge. We have analyzed the effect of this charge and the exchange interaction of electrons on the potential shape of the wire and the conductance. Under far from equilibrium condition we predict the possibility for several stable states to appear at a given external voltage.

Introduction

Recent experiments and theoretical investigations of coherent transport in semiconductor quantum wires (QW) have clearly shown that observed transport properties are significantly determined by the exchange interaction of electrons [1], and by the presence of electron reservoirs, to which the QW is coupled [3, 2]. Previously [4] we have shown that the strong effect of reservoirs on electron transport appears as a result of the electron density redistribution between the QW and the reservoirs and the charging of the QW. In the present paper we investigate the charging effect on the electron transport taking into account the exchange interaction of electrons with the use of the model [4, 5] based on the Hartree-Fock approximation.

The electron transport and the distribution of the electron density and the potential are investigated considering a QW and reservoirs as a unified system. We show that the chemical potentials of uncoupled QW and reservoirs are essentially different. When a QW and reservoirs are brought into the contact, the electron density is redistributed between the QW and the reservoirs. As a result the QW acquires the net charge and contact potential difference appears which affects electron transport. The acquired charge changes the linear conductance of a QW with non-adiabatic transition to reservoirs. However the most interesting consequence of a charge acquired in the QW is the instability that arises under a high enough applied voltage. The development of instability results in the appearance of multi-stabile states, *i.e.* in the existence of several stable states at a given voltage.

The exchange interaction gives rise to the increase in the Friedel oscillation potential near the non-adiabatic contacts. However the Friedel oscillations do not anywhere significantly suppress the conductance because the QW becomes inhomogeneous as a result of its charging. The essential effect due to exchange interaction is the lowering of the effective potential profile in the QW and correspondingly the increase in the electron density.

1. Contact potential difference

The decoupled QW and the electron reservoirs have their own chemical potentials which are generally not equal each other. The chemical potential is determined be the Fermi energy of non-interacting electrons and the self-energy $\Sigma(k_F)$ which contains the contributions arising from the exchange and correlation interaction as well as from the electron interaction with the positive background charge. We find the chemical potential difference $\Delta\mu$ between a QW and a reservoir. The results are illustrated in Fig. 1 for different Wigner–Seitz parameters r_s. It is seen that $\Delta\mu$ can be positive and negative, its magnitude being as high as several effective Rydbergs.

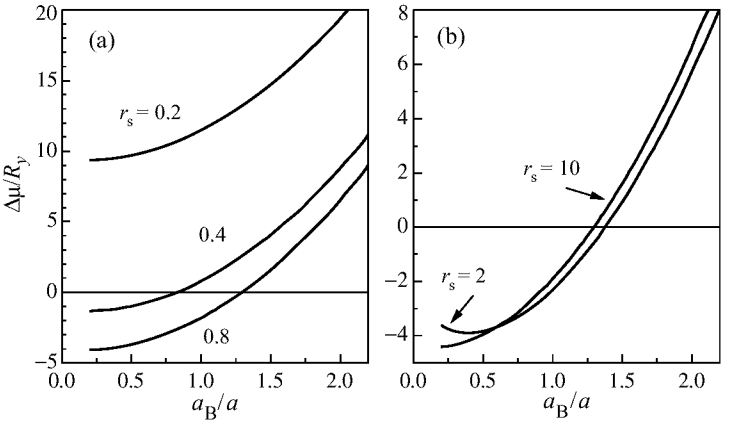

Fig. 1. Dependence of the chemical potential difference $\Delta\mu$ between the decoupled QW and the 2D electron reservoir on the wire radius a for various density parameters: (a) $r_s < 1$, (b) $r_s > 1$. R_y is effective Rydberg, a_B is the effective Bohr radius. The 2D layer thickness was put equal to the QW diameter, the density parameter of the 2D electrons R_s was equal to 0.5.

If the wire is now coupled to the 2D reservoir, the electron density is redistributed. The QW acquires the net charge and contact potential difference appears. In contrast to the similar phenomenon in the classical case of 3D conductors, there are two features: (*i*) the contact electric field is not screened over finite length but spreads over the length determined by the size of conductors; (*ii*) the spatial distribution of the electron density is governed by quantum mechanics.

The self-consistent calculation of the electron density distribution, electric potential and electric current were done using the model of our previous works [4, 5]

2. Linear conductance

The conductance is investigated in the case of non-adiabatic contacts between a QW and reservoirs. The linear DC conductance has been studied as a function of the chemical potential μ_0 in the system. The conductance oscillates with μ_0 because of the resonances of the electron waves over the QW length, L. The acquired charge (or the contact potential difference) leads to the change in the kinetic energy of electrons and in such a way affects the oscillation period.

The exchange interaction makes the conductance oscillations more frequent. The reason for this effect is that the exchange interaction results in an effective lowering of the potential energy of electrons and consequently in the increase of their kinetic energy. The

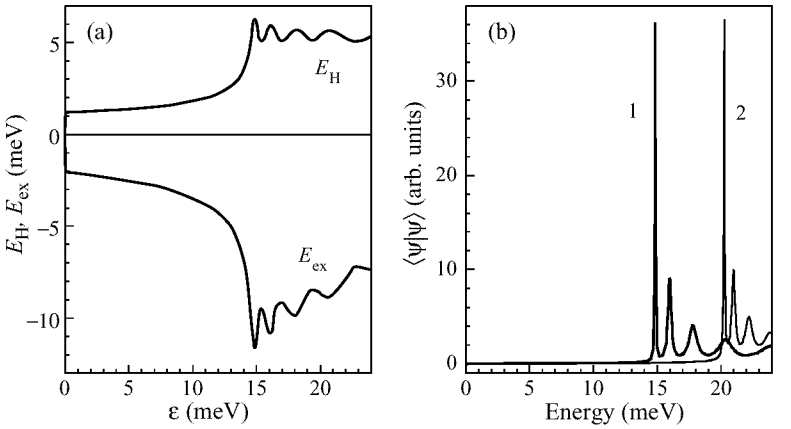

Fig. 2. (a) Average exchange (E_{ex}) and Hartree (E_H) energies of electrons incident on the QW with the energy ε. (b) The electron density spectrum averaged over the QW. Thick line (1) is obtained taking into account the exchange interaction. Thin line (2) is the Hartree approximation. The parameters used in the calculation are: $a = 5 \cdot 10^{-7}$ cm, $L/a = 30$, U_0=20 meV, $\mu_0 - U_0 = 4$ meV.

exchange interaction effect on the effective potential is illustrated in Fig. 2. Here the exchange interaction energy and the Hartree energy are compared. The exchange interaction is seen to diminish potential energy stronger than the Hartree energy increases it. Also shown is the spectral distribution of the electron density in the QW with and without the exchange interaction. Owing to the exchange interaction the electrons with energy below the transverse quantization energy U_0 can pass through the QW.

3. Non-linear transport and multi-stability

A significant redistribution of the electron density between the QW and the reservoirs occurs under far from equilibrium conditions arising when the applied voltage exceeds the Fermi energy. Electrons are injected from the left reservoir (cathode) while the electrons entering the QW from the positive reservoir (anode) are scattered back inside the QW. As

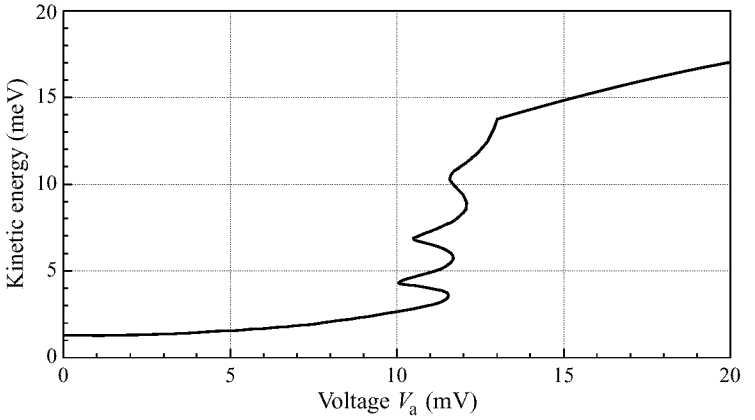

Fig. 3. Dependence of the average kinetic energy of electrons on the applied voltage. The calculations are for the following parameters: $a = 5 \cdot 10^{-7}$ cm, $L/a = 20$, $U_0 = 10$ meV, $\mu_0 - U_0 = 3$ meV.

a consequence the electron density decreases in the QW (roughly speaking to one-half of the equilibrium density) though the positive background charge is unchanged. Because the positive charge is dominant, a potential well appears in the QW, with the potential shape being distorted by the external potential.

When the applied voltage is high enough in comparison with the Fermi energy, the electron density and potential distribution becomes instable under the fixed voltage condition: there are several stable potential shapes and the system can switch between them. These potential shapes have the same potential difference between the QW ends, but differ each other by the depth and the shape of the potential well. A parameter that characterizes uniquely the nonequilibrium state is the mean kinetic energy of electrons in the QW. This parameter is shown in Fig. 3 as a function of the applied voltage V_a. The kinetic energy (and hence the potential energy as well) is seen to be multivalude at a given voltage.

Acknowledgements

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